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CONDENSED MATTER

Change in the Crystallization Features of Supercooled Liquid Metal with an Increase in the Supercooling Level

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The process of homogeneous crystal nucleation has been considered in a model liquid, where the interparticle interaction is described by a short-range spherical oscillatory potential. Mechanisms of initiating structural ordering in the liquid at various supercooling levels, including those corresponding to an amorphous state, have been determined. The sizes and shapes of formed crystal grains have been estimated statistically. The results indicate that the mechanism of nucleation occurs throughout the entire considered temperature range. The crystallization of the system at low supercooling levels occurs through a mononuclear scenario. A high concentration of crystal nuclei formed at high supercooling levels (i.e., at temperatures comparable to and below the glass transition temperature T_g) creates the semblance of the presence of branched structures, which is sometimes erroneously interpreted as a signature of phase separation. The temperature dependence of the maximum concentration of crystal grains demonstrates two regimes the transition between which occurs at a temperature comparable to the glass transition temperature T_g.

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In terms of thermodynamics, a supercooled liquid is in a state of unstable equilibrium, which results in the appearance of domains of a crystal phase in it [1–6]. At the same time, the character of the process of structural ordering should significantly depend on the conditions under which the supercooled state was formed, in particular, on the cooling rate of the liquid and on its final supercooling level $\Delta T/T_m = 1 - T/T_m$, where T_m is the melting temperature of the system [2, 7, 8]. At low and moderate supercooling levels covering the temperature range $T_g < T < T_m$, crystallization is usually initiated through the scenario of crystal nucleation, which is described within classical nucleation theory [1, 2, 8]. At temperatures below the glass transition temperature T_g, which correspond to high supercooling levels, the system forms an amorphous (glassy) state, where the space–time scales of crystal nucleation are beyond the sensitivity range of modern experimental instruments. Furthermore, an increase in the supercooling level of the amorphous system leads to an increase in the concentration of small crystal grains, the characteristics of the formation and growth of which cannot be predicted/described within classical nucleation theory [1]. For this reason, a commonly accepted complete understanding of the crystallization process of amorphous systems is still absent in spite of numerous studies [4, 9–12]. In particular, statements of the possibility of crystallization of liquids at high supercooling levels through the mechanism of phase separation are contradictory [13–15]. Some authors present signatures that can be considered as indications of the spinodal mechanism of structural ordering in single-component supercooled liquids [14], whereas other authors [15, 16] argue that the spinodal mechanism is impossible in these systems. The aim of this work is to consider this issue.

We consider a multiparticle system, where the interaction between particles is described by a short-range spherical oscillatory potential [17, 18], which effectively reproduces the ion–ion interaction in metal melts. This specific potential promotes the formation of a relatively stable amorphous state. The simulated system is shown in Fig. 1. We consider the temperature range $T = (0.5–1.4)\epsilon/k_B$ on the isobar $p = 15\epsilon/\sigma^3$, which corresponds to temperatures below the melting temperature of the system $T_m \simeq 1.72\epsilon/k_B$ and supercooling levels from $\Delta T/T_m \approx 0.19$ (at $T = 1.4\epsilon/k_B$) to ≈ 0.71 (at $T = 0.5\epsilon/k_B$) [18].[1] The glass transition temperature of the system is $T_g \simeq 0.78\epsilon/k_B$ (at the cooling rate $0.04\epsilon/(k_B T)$ on the isobar

[1] Physical quantities are given in Lennard-Jones units: the effective diameter of the particle σ, the energy unit ϵ, the time unit $\tau = \sigma\sqrt{m/\epsilon}$, where m is the mass of the particle; the temperature T and pressure p are measured in units of ϵ/k_B and ϵ/σ^3, respectively, where k_B is the Boltzmann constant.